

Effect of uniaxial pressure on the magneto-structural transitions of iron arsenide superconductors

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We study theoretically the variation of the magnetic and the structural transition temperatures of the iron arsenide superconductors with external uniaxial stress. We show that the increase of the transition temperatures reported in recent experiments is compatible with a simple magneto-elastic model in which the physical origin of this variation is linked to the fact that antiferromagnetic bonds are longer than the ferromagnetic ones in the magnetic phase. We make predictions which can be verified in order to test the relevance of this model.

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Introduction. At low doping, iron arsenide superconductors exhibit magneto-structural transitions from paramagnetic metals with tetragonal crystalline symmetry to low temperature antiferromagnetic metals with $(\pi, 0)$ magnetic order and orthorhombic crystal structure (using the notation of 1Fe/cell Brillouin zone) [1]. These transitions are either concomitant or close to one another, thereby suggesting the presence of non-trivial magneto-elastic coupling [2, 3]. The structural transition consists of a C_4 -symmetry breaking that, from a purely electronic point of view, can be seen as a nematic transition [4]. Consistent with this interpretation, various experiments have reported in-plane anisotropy of the electronic properties between the x - and the y - axes in the orthorhombic phase [5]. Since the study of such anisotropy is best performed using detwinned samples, experimental methods have been developed to perform the detwinning mechanically using in-plane uniaxial pressure [6]. However, an important prerequisite for interpreting these data is the understanding of how the magneto-structural transitions are themselves affected by the uniaxial pressure. Very recently experiments on BaFe_2As_2 , one of the most extensively studied systems for electron anisotropy, have shown that the both the structural and the magnetic transition temperatures, T_S and T_N respectively, are remarkably sensitive to uniaxial pressure [7, 8]. In fact, it has been reported that a modest compressive stress of 0.7 MPa along the shorter y -axis results in an increase of T_S by about 10 K, and that of T_N by few Kelvins [7]. Strikingly enough, tensile stress produces a similar increase of the magneto-structural transition temperatures [8]. This rules out a trivial magnetostriction effect because, in that case, compressive and tensile stresses are expected to give opposite (increase vs. decrease) results.

The purpose of this paper is to point out that these changes in T_S and T_N can be understood quite readily as a consequence of magneto-elastic coupling. Specifically, of the coupling that in the magnetic phase ensures that the antiferromagnetic bonds are longer compared to their ferromagnetic counterparts, a feature which is

universal to all known iron based superconductors [1]. The magnitudes of the above changes are expected to increase if the system is near a second order orthorhombic instability, which is the case of BaFe_2As_2 . As a corollary to these reasonings, we predict that applying tensile/compressive stress along the shorter/longer Fe-Fe bonds in the orthorhombic phase will, in fact, reduce the magneto-structural transition temperatures.

Theory. We write the free energy of the system as

$$F = F_M + F_E + F_{ME} - \sigma_{xx}u_{xx} - \sigma_{yy}u_{yy},$$

where σ_{ii} denotes external uniaxial stress, with the convention that $\sigma < 0$ for compressive stress and $\sigma > 0$ for tensile stress, and u_{ij} are the components of the in-plane strain tensor with $(i, j) = (x, y)$. The magnetic part of the free energy is given by

$$F_M = A (\mathbf{L}_+^2 + \mathbf{L}_-^2) / 2 + \dots,$$

where \mathbf{L}_+ and \mathbf{L}_- are magnetic order parameters corresponding to $(\pi, 0)$ and $(0, \pi)$ orders respectively, and $A = \alpha(T - T_N^0)$ where T_N^0 is the nominal Néel transition temperature. The elastic part is described by

$$F_E = \frac{K}{2} (u_{xx} + u_{yy})^2 + \frac{C_0}{2} (u_{xx} - u_{yy})^2 + \frac{B}{4} (u_{xx} - u_{yy})^4 + \dots,$$

where K is the bulk modulus, C_0 is the temperature (T) dependent orthorhombic elastic constant, and B is a temperature independent constant. The important magneto-elastic part is given by

$$F_{ME} = -g (u_{xx} - u_{yy}) (\mathbf{L}_+^2 - \mathbf{L}_-^2), \quad (1)$$

with the coupling constant $g > 0$ such that in the magnetic phase the antiferromagnetic bonds are longer than the ferromagnetic bonds (see below). The ellipses in the above equations denote terms that are not relevant for the current discussion. Since the systems of interest are

near a second-order structural transition where $C_0 \rightarrow 0$, magnetostriction effects are sub-dominant and can be ignored.

The coupling (1) has been shown to play a key role in establishing a universal phase diagram of these systems [2, 3]. In particular, the presence of tricritical points at which the magnetic transition changes character from first to second order were predicted for this phase diagram in [2], and it has later been confirmed experimentally in [9]. However, in the following we consider the case where the intrinsic instabilities (defined as the temperatures where the coefficients A and C_0 are zero) are sufficiently apart in T such that the magnetic transition remains second order and the elastic response to external stress is linear at T_N . For the sake of concreteness we treat the case where $T_S > T_N$ (which is relevant for BaFe_2As_2). In the absence of external stress the magnetic ordering takes place at

$$T_N(\sigma = 0) \equiv T_N(0) = T_N^0 + 2g\delta/\alpha,$$

where $\delta \equiv (|C_0|/B)^{1/2}$ is the spontaneous orthorhombic distortion that appears for $T < T_S$ due to the lattice instability ($C_0 < 0$). Note that $g > 0$ ensures that in the magnetic phase the antiferromagnetic bonds are longer than the ferromagnetic ones (mathematically, the $u_{xx} > u_{yy}$ and the $u_{xx} < u_{yy}$ solutions are coupled to the instabilities of \mathbf{L}_+ and \mathbf{L}_- respectively). In the following we describe two different experimental paths, namely stress applied above and below T_S (in the presence of finite stress T_S defines a cross-over where C_0 vanishes), and we assume that below T_S the system is in a single domain state with $u_{xx} > u_{yy}$.

(i) *Uniaxial stress applied in the paramagnetic tetragonal phase.* We consider uniaxial stress σ along one of the two equivalent directions, say y - for concreteness as in [7]. The strains induced by σ are obtained by minimizing the total free energy $\frac{\partial F}{\partial u_{ij}} = 0$. Since we are assuming that the system first feels the underlying structural instability and then undergoes the magnetic transition ($T_S > T_N$), it is convenient to carry out this minimization by expressing the total strain as $u_{ij} \rightarrow u_{ij}^0 + u_{ij}$, where u_{ij}^0 represent the strains that would appear spontaneously due to the structural transition at T_S ($u_{xx}^0 - u_{yy}^0 = \pm\delta$). In this way, the change in the effective orthorhombic elastic constant $C_0 \rightarrow \tilde{C}_0 = 2|C_0|$ that takes place below T_S is captured via u_{ij}^0 . Sufficiently below T_S the elastic response is linear and the strains induced by σ read $u_{yy} = -(K + \tilde{C}_0)/(K - \tilde{C}_0)u_{xx} = \sigma(K + \tilde{C}_0)/(4K\tilde{C}_0)$. Substituting these expressions back in the free energy we find that the effective magnetic energy is modified to $F'_M = F_M + g\sigma(\mathbf{L}_+^2 - \mathbf{L}_-^2)/(2\tilde{C}_0)$. The Néel temperature is determined by the leading instability between \mathbf{L}_+ and \mathbf{L}_- associated to $(\pi, 0)$ and $(0, \pi)$ orders respectively. In the case of compressive stress the $(\pi, 0)$ magnetic state is promoted, while with tensile stress it is the $(0, \pi)$. But for

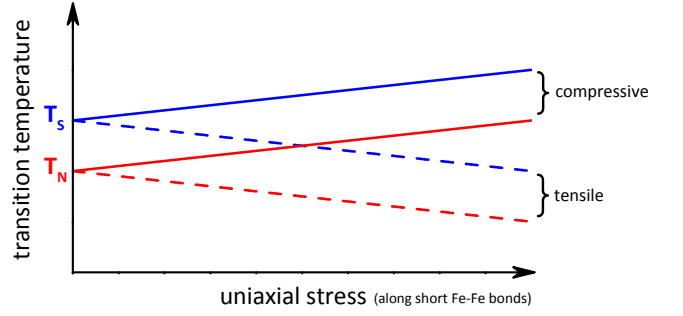


FIG. 1: (Colour online). Schematic variation of magnetic and structural transition temperatures, T_N (red) and T_S (blue) respectively, with uniaxial stress in detwinned samples. According to Eq. (2) T_N increases, and T_S tracks it (solid lines), for both compressive and tensile stress applied in the tetragonal phase as seen experimentally [7, 8]. Eq. (3) predicts that T_N decreases, and T_S tracks it (dash lines), for tensile/compressive stress applied along the short/long Fe-Fe bonds in the orthorhombic phase.

both compressive as well as for tensile stress T_N increases as

$$T_N(\sigma) = T_N(0) + \frac{g|\sigma|}{\tilde{C}_0\alpha}. \quad (2)$$

Note that this conclusion is also valid for systems where the intrinsic Néel transition appears before the structural one (i.e., $T_N^0 > T_S$), with \tilde{C}_0 replaced by C_0 in Eq. (2).

(ii) *Uniaxial stress applied in the paramagnetic orthorhombic phase.* In the single-domain state with $u_{xx} > u_{yy}$, which promotes the $(\pi, 0)$ magnetic order, the uniaxial stress can be applied either along the long or the short directions (x and y respectively). The induced strains can be obtained by minimizing the total free energy as before. After substituting the resulting expressions back in the free energy we find that stress applied along the short y direction shifts the Néel temperature to

$$T_N(\sigma) = T_N(0) - \frac{g\sigma}{\tilde{C}_0\alpha}. \quad (3)$$

Thus, while T_N increases in the case of compressive stress, it actually decreases in the case of tensile stress unlike in the previous case (i). Obviously, the conclusion is reversed if the stress is applied along the long x -direction.

Discussion. Eqs. (2) and (3) are the main results of this paper, which are illustrated in Fig. 1. Note that these results are a direct consequence of the magnetoelastic coupling described by (1) and symmetry considerations. As such, they do not depend upon whether the magnetic excitations are more itinerant-like or more localized-like. Furthermore, it can be argued that these conclusions remain unchanged even if the C_4 -symmetry breaking is due to electron spin nematicity or due to orbital ordering (in which case orthorhombicity is a secondary order parameter). The linear increase of T_N with both compressive

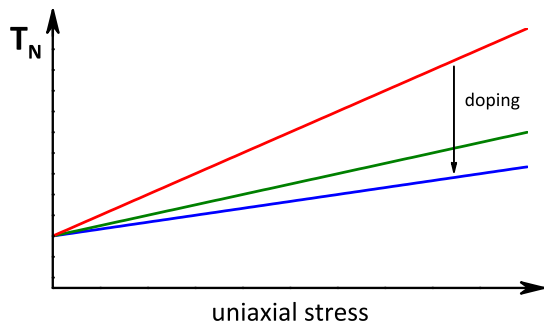


FIG. 2: (Colour Online). Schematic variation of the magnetic transition temperature T_N with uniaxial stress σ for different dopings. The slope $dT_N/d\sigma$, which is inversely proportional to $|T_S - T_N|$ in the current theory, is predicted to decrease with doping.

and tensile external stress described by Eq. (2) has been observed experimentally for small σ [7, 8]. Note that the sign of g is crucial for understanding these experimental findings. The decrease of T_N with compressive/tensile uniaxial strain applied along the long/short Fe-Fe bonds described by (3), on the contrary, is a prediction to be confirmed in future experiments. In fact, in the case where the system is not completely detwinned, the applied stress reduces the Néel temperature of the “wrong” domains compared to that of the “correct” ones, and this results in the smearing of the experimentally determined T_N . Furthermore, since the orthorhombic elastic constant C_0 appears in the denominator in both Eqs. (2) and (3), closer the system is to a second order orthorhombic instability as in BaFe_2As_2 and EuFe_2As_2 [10], larger is the variation of T_N with σ . On the contrary, we expect the magneto-structural transitions to be relatively insensitive to σ for CaFe_2As_2 and SrFe_2As_2 for which the structural instability is first order. In fact, if we assume that at the Néel transition C_0 varies linearly with temperature as $C_0 \propto T - T_S$, then we get that the slope $dT_N/d\sigma$ varies inversely with $(T_S - T_N)$. This conclusion can in principle be tested by comparing the results for samples at various doping as illustrated in Fig. 2.

Finally, we focus on the variation of T_S with external uniaxial stress. It has been pointed out that the orthorhombic transition can be interpreted as a result of structural softening due to magnetic fluctuations that develop near a $(\pi, 0)$ magnetic order [11, 12]. This interpretation provides a simple explanation why T_S and T_N track each other in the temperature-doping phase diagram of all the iron arsenides. More concretely, if we assume that the structural transition occurs in a regime where the magnetic fluctuations are controlled by the magnetic quantum critical point, we get that the correction to the orthorhombic elastic constant is [11] $\delta C_0 = -\Lambda \ln[T_0/(T - T_N)]$, where Λ and T_0 are constants that depend on microscopic details. The condition

$C_0 + \delta C_0 = 0$ determines the structural transition point, from which we obtain

$$T_S = T_N + T_0 e^{-C_0/\Lambda}. \quad (4)$$

Thus, we expect T_S to increase (or decrease) with σ in order to keep track of the increase (or decrease) of T_N . Note that this conclusion is qualitatively valid even if the magnetic fluctuations are controlled by the finite temperature magnetic critical point.

Conclusions. We have studied the variation of the magneto-structural transition temperatures of the iron arsenide systems with uniaxial stress. We have shown that the physical origin of this variation is the magneto-elastic coupling which makes the antiferromagnetic bonds longer than the ferromagnetic ones in the magnetic phase. The conclusions of the theory are compatible with the current experimental findings. The magnitude of this variation is relatively large because of the proximity of the orthorhombic instability, which is the case of BaFe_2As_2 (and presumably also of EuFe_2As_2). In order to test this interpretation we predict that (i) the transition temperatures will decrease if, after preparing the sample in a single-domain state, tensile/compressive stress is applied along the shorter/longer Fe-Fe bonds in the orthorhombic phase, (ii) and that the slope $dT_N/d\sigma$ is inversely proportional to $|T_S - T_N|$ when the two transitions are close enough (but not too close to make the magnetic transition first order). Note that our results are independent of microscopic details concerning the magnetic properties of the iron arsenides.

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Note added. Hu *et al.* [13] have also studied pressure effects in iron-pnictides from a microscopic spin model and a pure electron-nematic point of view. Their results are compatible with Eq. (2).

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